CHEM 2P20 SciFinder-n Exercise

The objective of this exercise is to gain experience exploring the chemical literature; register and use Brock's SciFinder-n database; learn how to create citations using ACS Style; explore chemical naming, structure drawing, reaction and database searching strategies; and, be better informed of Brock University chemists' research interests, productivity and expertise.

Go to the Brock Library Chemistry Research Guide to identify most-often used open and proprietary books/ebooks, web resources and scholarly databases. https://researchguides.library.brocku.ca/CHEM

Go to the SciFinder-n database link under the Chemistry Research Guide articles tab or the Brock Library list of databases and click on "register" for an account. This requires you to move through the Brock proxy server and create a unique SciFinder-n username and password. This registration is time limited so follow up with email authentication asap. This account is yours and is different from your Brock proxy username/password. Once you have an account for SciFinder-n remember to use your Brock proxy username/password and then your unique SciFinder-n username/password to access this database. This SciFinder-n access is yours as long as you are a member of the Brock University community.

Go to the Chemistry Department web site to review faculty and their research group's publications and activities. https://brocku.ca/mathematics-science/chemistry/directory/

Select **one** of the following Brock Department of Chemistry faculty member that specializes in organic chemistry from the following names: **Dudding, Duncan, Metallinos, Atkinson, Yan, or Zelisko**. Scan these faculty research groups' web site, list of publications, profile, review their interests, and do a bit of browsing before selecting your faculty member for this assignment.

Complete these ten questions using this form to get you thinking about scholarly research, chemistry and adding value to your learning.

Add your name and student number: _____

1. Name the researcher to be used for this exercise writing out variations in the spelling of their first/last name and/or initials that are often used in publications (this is really important!):

   _____

   Does this researcher have an ORCiD iD? https://orcid.org/

   Yes/no (If so please include the ORCiD URL and link, note whether it is open to the public)

   _____

   Have you registered/created a personal ORCiD ID?

Yes/no, If yes, indicate below, if not, do it today, it is free and list below!

2. Consult this faculty members research interests and publications to document keywords and phrases that best describe 1) chemistry subject areas / topics researched 2) substances/types/classes of chemical compounds investigated and 3) varying instrumentation, experimental equipment used as it relates to bio/synthetic/organic chemistry:

    1. _____
    2. _____
    3. _____

3. Follow instructions on the Brock *Library Chemistry Research Guide* under the "Articles" tab to register for a SciFinder-n account, confirm registration by e-mail authentication, and sign into the SciFinder-n database. Create a screen shot of your SciFinder-n account search engine page below that includes your personal name located on this databases entry point to confirm that you have an account:

4. Search SciFinder-n by References to search for publications by your selected Researcher/*Author Name*. Be sure that your researcher/faculty member is the same person that is currently affiliated with Brock University noting that researchers use one or two initial and/or their full name and initial(s) to differentiate themselves, and other systems including ORCIC IDs.

    a. SciFinder-n number of references for this researcher (remember initials, names, etc.):

    _____

    b. Filter/limit search results for this researcher to find the number of CAplus (Chemical Abstracts) references:

    _____

    c. Filter References by Document Type = Journal, Language = English, and sort citations by Publication Date: Newest, to find the number of English language scholarly peer-reviewed articles:

    _____

    d. Filter and sort at will to find one recent article of interest that is somewhat connected with the work of this organic chemistry course. Cite this single article using ACS Style:

    _____

    Read it, does it make sense, check out the substances, reactions, acknowledgements, references… create and paste a screen capture of the article's first page into this assignment:

e. For this SciFinder-n article record the number of unique author keywords (if available):

_____

f. For this SciFinder-n article record the number of database concepts:

_____

g. For this SciFinder-n article record the number of unique substances (if available):

_____

h. For this SciFinder-n article select one **organic compound** that is of personal interest, and **has enough references, reactions and suppliers to be noteworthy**. Document the CAS Registry Number you have chosen:

_____

5. Chemical structure searching. This is important for organic chemistry and related disciplines. Start a new search and click on SciFinder-n search for Reactions. There are several ways of doing this, click on the SciFinder-n Reactions option, click on the "Draw" icon and insert your CAS Registry number from question 4h. Click on the T search icon next to it, click off to just get the structure and click off "the Click and drag objects…" note. Also note that you can add substances/ structures, short cuts, compounds, reaction sequences… to create a unique structure searching reaction question… For this exercise just click OK. Then click the search icon next to the Draw icon when ready.

   How many substances were found for this drawn structure?

   _____

6. Please provide the IUPAC name, registry number and molecular formula (using the Hill system) for your compound identified in question 4h:

   IUPAC chemical name(s): _____
   CAS Registry Number: _____
   PubChem CID: _____
   molecular formula: _____

   Copy, cut and paste, or using a chemical drawing software e.g. ChemDraw or create a screen shot of an image or picture of your substance's chemical structure below:

   Molecular or chemical formulas are never easy to create, especially for complex, biomolecular, pharmaceuticals, theoretical and trade compounds.

There are many different naming conventions, styles and practices. CAS including SciFinder-n build on a specific naming system that is an industry standard, but there are variant names for chemicals, PubChem is another naming convention and open database, see if you compound is found in this database. The Brock Library Chemistry Research Guide is a resource for chemistry and related disciplines, click on the "Chemicals / Drugs" tab to find alternate and open naming databases.

For this SciFinder-n substance, click on Reactions, filter or limit by Substance Role: Product.

How many reactions as a product are documented in this database?

_____

Browse these reactions noting that you can further limit by several variables related to reaction sequences, database filters, document types including journal articles and patents… and sort by several means including relevance, currency, number of steps, yield… and remember that each reaction is cited by at least one scholarly source.

Cite a relevant journal article, then filter by document type: patent - to find a patent. Cite both using ACS Style, (if you can't find a patent then just cite a second article):

_____

_____

Note the use of Zoterobib to cite using ACS Style and check out the ACS Quick Style Guide for formatting different types of citations which is Part 4.3 in the ACS Guide to Scholarly Communication.

7. Scholarly Peer Review. Determine whether the article(s) you cited in the previous question is/are peer reviewed.

   What's Peer Review (Brock Library, YouTube, 1:33),

   Are these articles peer reviewed?

   Yes/no

   How do you know?

   _____

8. Comment: How might accessing SciFinder-n or equivalent scholarly databases help you in this course?

   _____

9. Comment: One thing you learned about the nature of your faculty member's research profile through this exercise?

_____

10. Comment: One thing new you learned about SciFinder-n, chemistry databases, and the nature of chemical information through this exercise?

_____

Help is always available from the Brock Library using Chat with a Librarian, emailing the library using libhelp@brocku.ca, book a research consultation, talking with your lab advisor/TA, talking with colleagues, connecting with chemistry experts when appropriate using help@cas.org and consulting with any number of disciplinary research guides by program, and the Brock Library Chemistry Research Guide.

Don’t forget to sign out of SciFinder-n when done and don’t share your unique login/password.